

Level statistics for quantum k -core percolation

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Quantum k -core percolation is the study of quantum transport on k -core percolation clusters where each occupied bond must have at least k occupied neighboring bonds. As the bond occupation probability, p , is increased from zero to unity, the system undergoes a transition from an insulating phase to a metallic phase. When the lengthscale for the disorder, l_d , is much greater than the coherence length, l_c , earlier analytical calculations of quantum conduction on the Bethe lattice demonstrate that for $k = 3$ the metal-insulator transition (MIT) is discontinuous, suggesting a new universality class of disorder-driven quantum MITs. Here, we numerically compute the level spacing distribution as a function of bond occupation probability p and system size on a Bethe-like lattice. The level spacing analysis suggests that for $k = 0$, p_q , the quantum percolation critical probability, is greater than p_c , the geometrical percolation critical probability, and the transition is continuous. In contrast, for $k = 3$, $p_q = p_c$ and the transition is discontinuous such that these numerical findings are consistent with our previous work to reiterate a new universality class of disorder-driven quantum MITs.

I. INTRODUCTION

With the exception of transition metal compounds, there exist two conventional paradigms for metal-insulator transitions (MITs): a Mott-Hubbard-type transition and an Anderson-type transition. The former is a consequence of tuning the interactions between electrons by changing the distance between atoms, for instance, and the MIT is discontinuous [1]. The latter is a consequence of the tuning the disorder in the material, and the MIT is continuous [2, 3]. Recently, a discontinuous disorder-driven MIT has been predicted for a model in which there exists geometric constraints on the disorder [4]. The model has been dubbed quantum k -core percolation. Quantum $k = 0$ -core percolation, or quantum percolation (QP), has been studied since the 1980's and exhibits a continuous, Anderson-type MIT [5, 6]. Quantum percolation is defined accordingly. Consider a lattice whose bonds are occupied independently and at random with bond occupation probability p . An electron can only hop between lattice sites i and j along an occupied bond and cannot hop along an unoccupied bond. In addition, there exists a constant on-site binding energy which is set to zero for convenience. In total, the tight-binding Hamiltonian for quantum percolation is

$$H = \sum_{i,j} t_{ij} a_i^\dagger a_j + h.c. \quad (1)$$

in which,

$$t_{ij} = \begin{cases} 1 & \text{with probability } p \\ 0 & \text{with probability } 1 - p \end{cases} \quad (2)$$

and a_i^\dagger and a_i are electron creation and annihilation operators.

Quantum percolation exhibits a MIT as p is increased from zero, at least for three dimensions and above [7–9]. In two dimensions, some studies indicate a transition [10–14], while others do not [15, 16]. Analytical work on the Bethe lattice indicates that the quantum percolation transition may be in the same universality class as geometric percolation except with the transition probability p_q above which there exists extended zero-energy wavefunctions is greater than the threshold above which there exists a spanning cluster, p_c [17, 18]. The geometric percolation transition is a continuous and, therefore, so is the quantum percolation transition presumably.

Recently, we have studied quantum k -core percolation on the Bethe lattice [4]. The term k -core refers to a geometrical constraint where every occupied bond must have at least $k - 1$ occupied neighboring bonds [19–24]. Such a geometric constraint may have implications for glassy systems [25], jamming systems [23], and even biological systems [26]. To enforce this constraint, bonds are initially occupied independently and at random with probability p . Then, those occupied bonds with less than $k - 1$ occupied neighboring bonds are rendered unoccupied. This removal procedure proceeds recursively throughout the lattice until all occupied bonds satisfy the k -core constraint. See Fig. 1 for an example on the Bethe lattice. For $k \geq 3$, the geometric percolation transition is in a different universality from ordinary geometric percolation with, for example, the fraction of occupied bonds in the spanning k -core cluster, P_∞ , scaling with p as $P_\infty = P_0 + P_1(p - p_c)^{1/2}$ for $p \geq p_c$ (with $p_c - p \ll 1$) where P_0 and P_1 are constants and p_c is the critical occupation probability for classical (geometric) percolation. This result is to be contrasted with

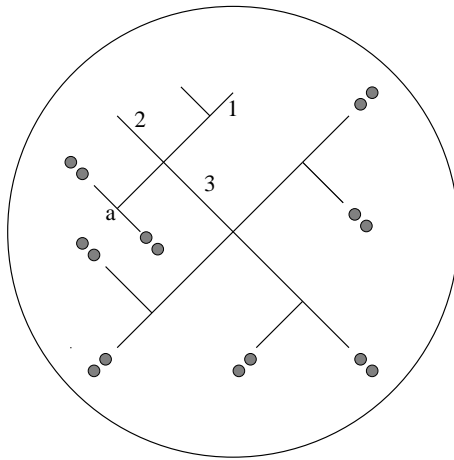


FIG. 1: Here $k = 3$ and $z = 4$. The shaded circles denote branches that are $k - 1$ connected to infinity. The removal of bonds 1 and 2 eventually triggers removal of bond 3 and bonds emanating from vertex a, including the shaded circles. The remaining three branches emanating from the center site survive the removal process.

$P_\infty \propto (p - p_c)$ for $p \geq p_c$ just above the transition for $k = 0, 1$. In other words, the geometric percolation transition is a random first-order transition, i.e. a discontinuous transition with several diverging lengthscales.

Once the k -core constraint has been implemented, we then impose the quantum percolation property that electrons can only hop along occupied bonds and compute the quantum conduction through the system self-consistently after assuming that the electronic wavefunction randomizes between bonds, i.e. the lengthscale of the disorder, l_d , is much greater than the coherence length, l_c . Within this scheme, for $k = 0, 1$, the model reduces to ordinary quantum percolation. In this case, we found that $1 > p_q > p_c$, where p_c signals the onset of the geometric percolation transition and p_q signals the onset of quantum conduction. We also found a random first-order transition for $k > 2$, and that interestingly enough, the critical threshold is the same as k -core geometrical percolation critical point. This transition should be contrasted with the Anderson-type MIT, which yields a continuous transition as does the quantum percolation transition on the Bethe lattice.

In this work, we numerically investigate the level statistics of quantum k -core percolation to compare with our previous analytical results on the Bethe lattice obtained in the limit $l_d \gg l_c$. In other words, how robust are our previous results in identifying a new universality class of disorder-driven MITs? Level statistics and its roots in random matrix theory is an important tool for studying universality, for example [27]. Correlations between energy eigenvalues of an individual quantum particle in a random potential in the conductive regime agrees with results from Gaussian matrix ensembles [28]. In the localized regime, correlations between the energy eigenvalues are absent and the level statistics become Poissonian. Right at the MIT, however, the level statistics are distinct from Gaussian matrix ensembles [29]. While these results pertain to the Anderson model where the disorder is on-site, the same analysis has been applied to quantum percolation on a cubic lattice, where the disorder is off-diagonal, and similar results have been found [30]. In fact, the critical exponent for the divergence of the localization length extracted from the level statistics analysis is somewhat consistent with the Anderson model. Therefore, we will implement a similar numerical analysis for quantum k -core percolation on a Bethe-like lattice to go beyond our previous approximation [4].

We, however, will not investigate the level statistics of quantum k -core percolation on finite-dimensional lattices for now. It turns out that k -core percolation on finite-dimensional lattices either exhibits properties of $k = 0$ geometric percolation or no transition. See, for example, Ref. [31]. One has to invoke more sophisticated constraints to observe different universal behavior from $k = 0$ geometric percolation [32] and so we expect the quantum behavior to be similar to quantum percolation for finite-dimensional lattices, though this conjecture should ultimately be tested.

The paper is organized as follows. We review the methodology and results for quantum percolation on the cubic lattice [30] as a means for calibration and then present our results for quantum $k = 0$ -core percolation and quantum $k = 3$ -core percolation on a Bethe-like lattice. We conclude with a discussion of the implications of our results.

II. QUANTUM PERCOLATION ON THE CUBIC LATTICE

First, we analyze the level statistics for quantum percolation on the cubic lattice. To do so, we diagonalize the Hamiltonian defined by Eqs. 1 and 2 on the cubic lattice of length L with periodic boundary conditions to obtain a

sequence of eigenvalues. This sequence is calculated for different realizations and increasing system sizes. The average density of states (DOS) for $L = 15$ as a function of occupation probabilities is presented in Fig. 2. The sharp peaks are due to small disconnected structures as discussed in Ref. [30]. Now, one can apply the various measures of level statistics only if the density of states is smooth. There exists a smooth energy range around 0.4. The eigenenergies near this range are then arranged from highest to lowest and the nearest-neighbor level spacing, S , is calculated and subsequently normalized by the average nearest-neighbor level spacing, i.e. normalized level spacing is denoted by $s = S / \langle S \rangle$.

One can then study the probability distribution for these level spacings, $P(s)$, as a function of p and L . When the system is in the insulator regime, the eigenfunctions are localized and, therefore, do not interact with each other such that $P(s)$ is Poisson distributed, i. e. $P(s) = e^{-s}$. When the system is in the metallic regime, Altshuler and Shklovskii [28] argued that if the width of the energy band of a sample $E < E_c \equiv \hbar D / L^2$, where L^2 / D is the characteristic time for an electron to diffuse through the sample, then the Hamiltonian of the system is characteristic of Gaussian Orthogonal Ensemble (GOE) in the absence of a magnetic field or spin-orbit scattering. More specifically, $P(s)$ obeys the Wigner-Dyson distribution, $P(s) = \frac{\pi s}{2} \exp(-\frac{\pi}{4}s^2)$. The cubic conductance $\langle G \rangle = \frac{e^2}{h} \langle N(E_c) \rangle = \frac{e^2}{h} \frac{E_c}{\langle S \rangle}$ tends to infinity when $L \rightarrow \infty$ in the metallic regime, thus $E < E_c$ is satisfied, and the level spacing distribution obeys the Wigner-Dyson distribution for the GOE.

The plot of $P(s)$ as function of bond occupation probability for $L = 15$ and an energy range of $[0.2, 0.6]$ is displayed in Fig. 2. It can be seen that the expected transition from Wigner-like behavior for large p to Poisson behavior for small p . Note that all curves intersect at $s \simeq 2$ as observed in the Anderson model [29]. Other energy ranges studied yielded similar results. A convenient way to obtain the critical exponent ν , characterizing the diverging localization length at the transition, is to study the parameter, γ , defined as

$$\gamma = \frac{\int_2^\infty P(s) ds - e^{-\pi}}{e^{-2} - e^{-\pi}}, \quad (3)$$

which characterizes the transition from Wigner to Poisson as p is decreased. Note that γ should increase from 0 to 1, as $P(s)$ goes from Wigner to Poisson. Denoting $\xi(p)$ as the localization length (such that $\xi(p) \sim (p - p_q)^{-\nu}$), the above parameter is expected to demonstrate scaling behavior, $\gamma(p, L) = f[L/\xi(p)]$. In the vicinity of the critical quantum bond probability p_q ,

$$\gamma(p, L) = \gamma(p_q, L) + C \left| \frac{p}{p_q} - 1 \right| L^{1/\nu}, \quad (4)$$

where C is a constant.

Figure 3 plots γ as a function of p around p_q for increasing L . The curves intersect near a single point given by $p_q \simeq 0.334$. This result is consistent with the result in Ref. [30]. The single crossing point indicates that there exists a metal-insulator transition and one can apply the scaling collapse suggested above. The optimal scaling collapse shown in Fig. 3 yields $\nu = 1.6 \pm 0.05$, which should be compared to 1.32 ± 0.08 obtained in Ref. [30]. Our latest result is even closer to the Anderson result than the previous work, where the most precise measurement is $\nu = 1.58 \pm 0.02$ [33].

III. QUANTUM k -CORE PERCOLATION ON A BETHE-LIKE LATTICE

Following the procedure presented in Ref. [34], a Bethe-like lattice is numerically created by first considering a one-dimensional ring with N sites such that each lattice site has two bonds emanating from it. Next, additional bonds are constructed between different lattice sites at random. The number of random pairs connecting different lattice sites depends on the fixed coordination number, z . More specifically, there must be z bonds per site. See Fig. 4 as an example for $z = 3$. As N increases, the average number of loops of length l increases as $(z - 1)^l$ such that the fraction of all lattice sites belonging to any loop of length $\leq l$ for $l \ll \log(N)/\log(z - 1)$ is negligible. Therefore, the structure becomes increasingly tree-like as N increases and no surface effects that have to be dealt with, which occurs when one performs numerical simulations on the Bethe lattice.

A. $k = 0$

For $k = 0$, A. B. Harris [18] gave a theoretical prediction of p_q on the Bethe lattice. One must simply solve $1 + (p_q \sigma^2)^{-1} = (p_q \sigma)^{2/(\sigma-1)}$ with $\sigma = z - 1$. By solving Harris's self-consistency equation above for $z = 6$, $p_q = 0.265$.

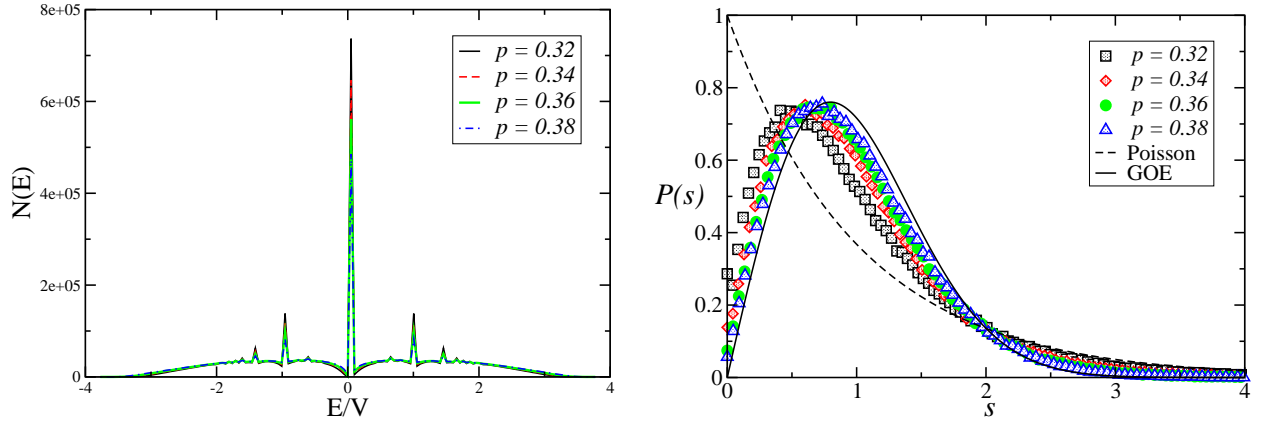


FIG. 2: Left: The DOS for $L = 15$ and different bond occupation probabilities. Right: $P(s)$ for $L = 15$ for different p s. The Wigner and Poisson forms are also shown.

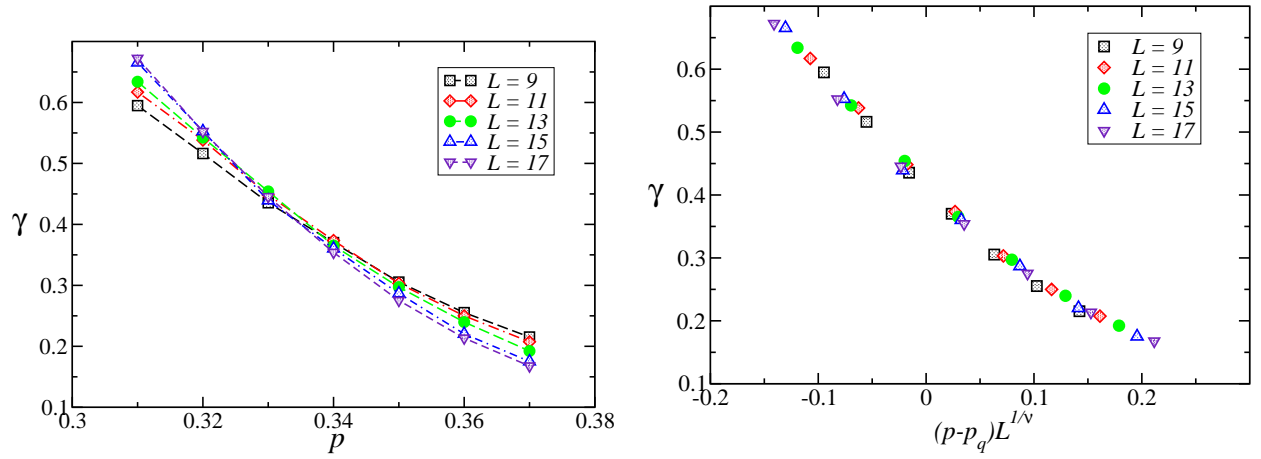


FIG. 3: Left: The function $\gamma(p, L)$ for different system sizes. Right: Scaling collapse for the cubic lattice.

We can test this result numerically with the level statistics analysis. Figure 5 plots $P(s)$ for different p s with $N = 1024$, $z = 6$ and an energy range of $[0.3, 0.8]$. Figure 6 plots $\gamma(p, N)$ for $z = 6$. The curves intersect near $p \sim 0.3$, which is close to the analytical result for the Bethe lattice, though the agreement is not precise. This difference between the analytical calculation and our numerical calculation is presumably due to the nature of the lattice such that the quantum mechanics is much more sensitive to loops than geometric percolation. To test this notion, when measuring the onset of geometric percolation on the Bethe-like lattice, we do arrive at good agreement between the analytical result, $p_c = 1/(z - 1)$, and our numerical result.

Moreover, the crossing point in Figure 6 indicates that we can collapse the data by assuming that, instead of $\gamma(p, L) = f[L/\xi(p)]$ in the cubic lattice case, $\gamma(p, L) = f[N/N^*(p)]$, where N^* is a crossover size similar to the localization length in the three-dimensional case. In other words, $N^* \sim (p - p_q)^{-\nu'}$. Therefore, $\gamma(p, L) = f[N^{1/\nu'}(p - p_q)]$. It has been conjectured that $\nu' = d_u \nu_{MF}$, where d_u is the upper critical dimension and ν_{MF} is the mean field correlation length exponent [35]. For geometric percolation, $d_u = 6$ and $\nu_{MF} = 1/2$ such that $\nu' = 3$. To date, the upper critical dimension of quantum percolation is not known. Interestingly, the upper critical dimension for the Anderson model is potentially infinite such that the mean field correlation length scales with dimension d [36]. More precisely, $\nu = \frac{1}{2} + \frac{1}{d-2}$.

Figure 6 shows the optimal scaling collapse to yield the exponent $\nu' = 4.5 \pm 0.2$ assuming that $p_q = 0.300(1)$. If we assume $p_q = 0.265$, then we do not arrive at a good scaling collapse. Regarding ν' , if we assume the same mean field correlation length of $\nu_{MF} = 1/2$ as in classical $k = 0$ percolation, which is consistent with the previous work of A. B. Harris [18] showing that the mean field susceptibility for zero-energy eigenstates diverges with the same exponent as in the geometric percolation problem (with p_q replacing p_c), then we extract an upper critical dimension of $d_u = 9$.

If, on the other hand, the upper critical dimension is infinite as in the case of the Anderson model, then different analysis must be undertaken.

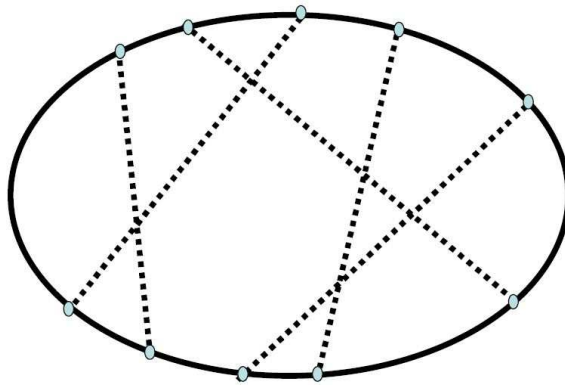


FIG. 4: An example of a Bethe-like lattice with coordination number, $z = 3$. Dotted curves indicate the random pairs.

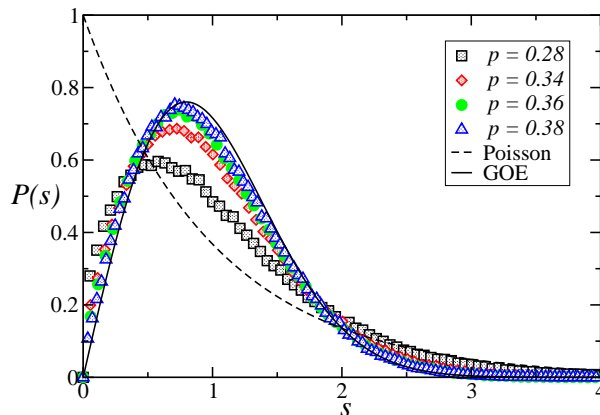


FIG. 5: $P(s)$ for the Bethe-like lattice for $N = 1024$ and $k = 0$ for different p s.

B. $k = 3$

In Ref. [4], we gave an example of a MIT driven by $k = 3$ -core disorder on the Bethe lattice with $z = 4$. More precisely, the quantum conduction as a function of occupation probability p is a random first-order transition with $p_q = p_c$. To obtain this result, we assumed that the phase randomized between levels on the Bethe lattice, i.e. $l_d \gg l_c$. Here, we use level statistics to test the robustness of our prior results. Since the geometric critical percolation occupation probability p_c is $8/9$, which is close to 1, we choose $z = 6, k = 3$, whose $p_c = 0.603$ [19, 22, 23]. Numerically, Figure 7 gives the fraction of remaining samples versus occupation probability, denoted by F , after applying the k -core constraint recursively for $z = 6, k = 3$. One can find that in a ideally infinite system size system, all occupied bonds are removed due to the k -core constraint for $p < 0.604$, while $p > 0.604$, occupied bonds remain. Note that $p_c = p_q = 0.604$ is quite close to the analytical p_c for $z = 6$ and $k = 3$ for the classical physics.

Figure 8 plots γ as a function of p for different system sizes. As the system size increases, larger error bars are shown for $p < p_c$, indicating less remaining occupied samples due to the k -core constraint. With no remaining occupied bonds for $p < p_c$, the system is insulating in a trivial sense and not in the sense that $\gamma \rightarrow 1$. What happens for $p > p_c$? The data indicates that γ tends to 0 as the system size increases for $p > p_c$, indicating that it is a metallic system. There is no crossing point above p_c such that p_c must equal p_q as we obtained previously. Note that we

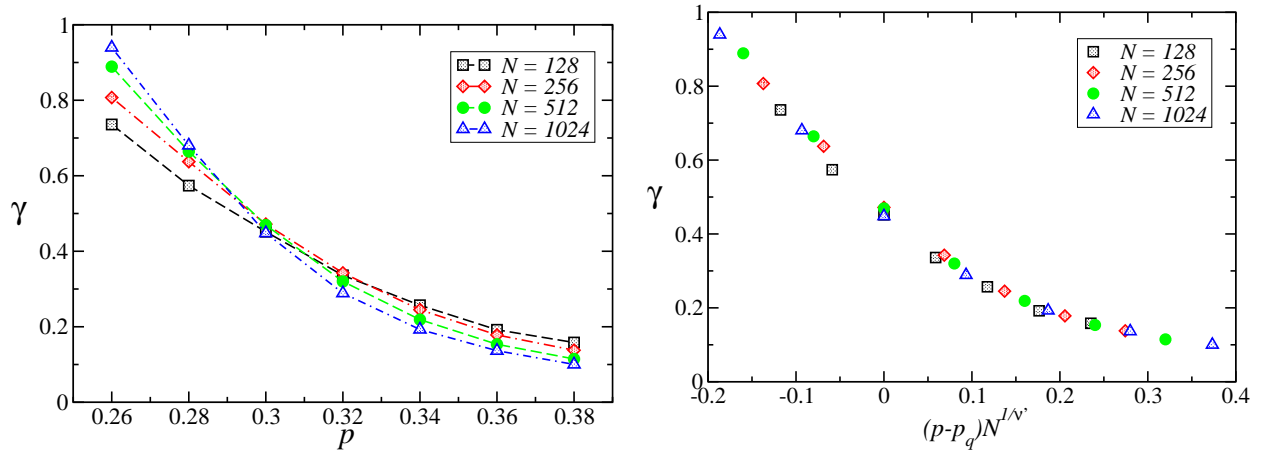


FIG. 6: Left: The function $\gamma(p)$ for different system sizes. Right: The scaling collapse for $\gamma(p)$.

could have observed a crossing point somewhere above p_c to indicate that $p_q > p_c$, but we do not. The data imply a discontinuous transition since γ tends towards zero as N becomes large for $p \geq p_q$.

IV. DISCUSSION

We have applied level statistics for quantum percolation on three different systems. The results on cubic lattice are consistent with the results from Ref. [30]. For quantum percolation on a Bethe-like lattice, we find a threshold probability that differs somewhat from Harris's Bethe lattice result [18]. This difference is due to the sensitivity of loops in quantum mechanics occurring in the Bethe-like lattice. Moreover, a scaling collapse with system size N yields a new critical exponent $\nu' = 4.5(2)$. Assuming the correlation length exponent is ν_{MF} is $1/2$, the same as the mean field result for geometric percolation, which is consistent with the Harris calculation [18], the upper critical dimension $d_u = 9$. We have also demonstrated the robustness of our previous work for quantum $k = 3$ -core percolation [4]. The level statistics here shows $p_q = p_c$, as before. In fact, for $p < p_c$, all bonds are removed and the system is an insulator, while for $p > p_c$, none of the bonds are removed and the system is conducting quantum mechanically. The data suggest that the system immediately goes to the Wigner-Dyson regime without going through a different regime at the transition, indicating a discontinuous transition, which also agrees with our previous work [4].

Therefore, our work provides an important counterexample for the Mott versus Anderson MIT paradigm, where

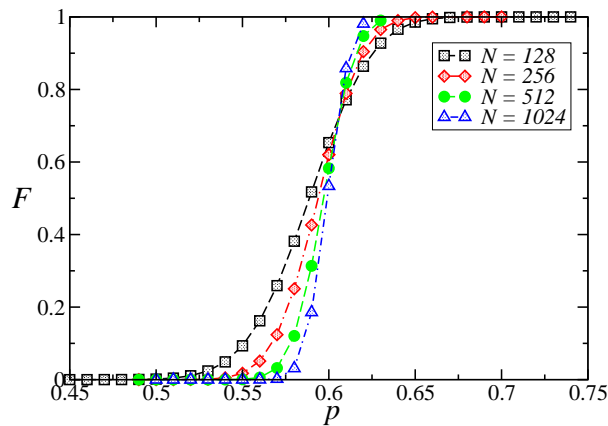


FIG. 7: Fraction remaining samples versus occupation probability after applying the k -core constraint, F , on the Bethe-like lattice for $z = 6$, $k = 3$.

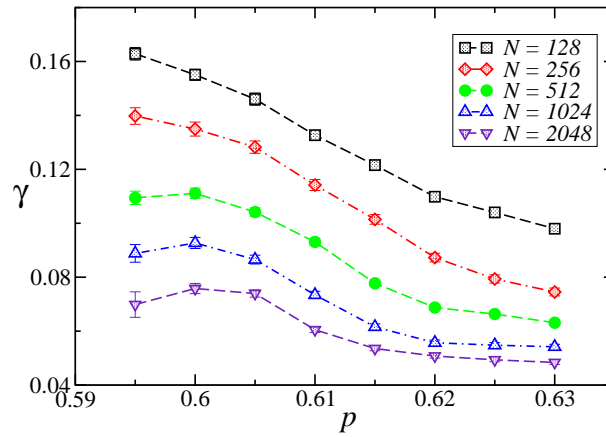


FIG. 8: γ as a function of p for different system sizes for the $z = 6, k = 3$ Bethe-like lattice.

disorder-driven (Anderson) MITs are continuous and interaction-driven (Mott-Hubbard) MITs are discontinuous. Our counterexample is due to the correlations in the disorder as a result of the k -core constraint. Correlations in the disorder have been shown previously to “complicate” matters. For instance, in one-dimensional wires with long-range, correlated disorder, there exists a MIT, which does not happen in the short-range, uncorrelated disorder case [37].

As for experimental implications, there are many experiments in the realm of classical transport on ordinary percolating systems. See, for example, Ref. [38] for a recent one on nanowire composites. In addition, transport in undoped graphene is linked to classical electronic transport on percolating networks, though quantum effects are also relevant [39]. However, can a quantum $k = 3$ -core percolation transition ever be realized? An experiment has already been conducted with a collection of silver quantum dots sitting atop of a Langmuir monolayer at room temperature [40]. As the interparticle spacing decreases by compressing the floating particles together, the electronic transport goes from hopping to tunnelling to ordinary metallic transport. The authors argue that disorder in the particle size and in the charging energy probably does not drive the transition and, instead, conjecture a possible first-order Mott transition at *room temperature*. However, in light of the analysis of the onset of classical conduction for $k = 3$ -core, where k encodes the scalar aspect of local mechanical stability in particle packings [23], we argue for a possible *classical* correlated percolation transition in conduction. Perhaps a quantum analog of this experiment can be realized in low-temperature packings of metallic nanoparticles to search for this new universality class of quantum disorder-driven MITs.

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